

# Discretization-related issues in the KPZ equation: Consistency, Galilean-invariance violation, and fluctuation–dissipation relation

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## Abstract

In order to perform numerical simulations of the KPZ equation, in any dimensionality, a spatial discretization scheme must be prescribed. The known fact that the KPZ equation can be obtained as a result of a Hopf–Cole transformation applied to a diffusion equation (with *multiplicative* noise) is shown here to strongly restrict the arbitrariness in the choice of spatial discretization schemes. On one hand, the discretization prescriptions for the Laplacian and the nonlinear (KPZ) term cannot be independently chosen. On the other hand, since the discretization is an operation performed on *space* and the Hopf–Cole transformation is *local* both in space and time, the former should be the same regardless of the field to which it is applied. It is shown that whereas some discretization schemes pass both consistency tests, known examples in the literature do not. The requirement of consistency for the discretization of Lyapunov functionals is argued to be a natural and safe starting point in choosing spatial discretization schemes. We also analyze the relation between real-space and pseudo-spectral discrete representations. In addition we discuss the relevance of the Galilean invariance violation in these consistent discretization schemes, and the alleged conflict of standard discretization with the fluctuation–dissipation theorem, peculiar of 1D.

## I. INTRODUCTION

Soon after its formulation in 1986, the KPZ equation [1–3]

$$\partial_t h = \nu \partial_x^2 h + \frac{\lambda}{2} (\partial_x h)^2 + F + \varepsilon \xi(x, t), \quad (1)$$

became a paradigm as the description of a vast class of nonequilibrium phenomena by means of stochastic fields. The field  $h(x, t)$  whose evolution is governed by this stochastic nonlinear partial differential equation, describes the height of a fluctuating interface in the context of surface growth processes in which it was originally formulated. In particular, Eq. (1) assumes a one-dimensional (1D) homogeneous substrate of size  $L$ . The parameter  $\nu$  determines the surface tension,  $\lambda$  is proportional to the average growth velocity (the surface slope is parallel-transported in the growth process), and  $F$  is an external driving force. Finally,  $\xi(x, t)$  is a Gaussian white noise with  $\langle \xi(x, t) \rangle = 0$  and  $\langle \xi(x, t) \xi(x', t') \rangle = 2\delta(x - x')\delta(t - t')$ . As usual, periodic boundary conditions are assumed.

From a theoretical point of view the KPZ equation has many interesting properties, like its close relationship with the Burgers equation [4] or with a diffusion equation with multiplicative noise, whose field  $\phi(x, t)$  can be interpreted as the restricted partition function of the directed polymer problem. But clearly, investigating the behavior of its solutions to obtain e.g. the critical exponents in one or more spatial dimensions [5–13] requires the (stochastic) numerical integration of a discrete version. Although a pseudo-spectral spatial discretization scheme has been recently put forward [14–16], as well as a numerical large deviation theory [4], real-space discrete versions of Eq. (1) are still largely used for numerical simulations [17–20], because of their relative ease of implementation and of interpretation in the case of non-homogeneous substrates (for instance, a quenched impurity distribution [21]) among other reasons. To that end, several real-space discretization schemes have been proposed [10, 11, 19], which are claimed to cure particular “diseases” of the numerical simulation.

In the present work, no attempt is made of comparing alternative real-space discretization schemes in sought of special KPZ features. Instead, we seek to point out some basic conditions that *any* spatial discretization must fulfill in order to consistently describe the KPZ equation. Nonetheless, for the sake of brevity and for ease of comparison with other

proposals, we shall adopt the notation in Ref. [19], namely (calling  $\Delta x \equiv a$ )

$$L = aN, \quad H_{j+k}^{j+l} \equiv \frac{h_{j+l} - h_{j+k}}{a},$$

$$L_j \equiv \frac{H_j^{j+1} - H_{j-1}^j}{a} = \frac{H_j^{j+1} + H_j^{j-1}}{a},$$

and

$$N_j^{(\gamma)} \equiv \frac{\left(H_j^{j+1}\right)^2 + 2\gamma H_j^{j+1} H_{j-1}^j + \left(H_{j-1}^j\right)^2}{2(1+\gamma)},$$

with  $\gamma \in [0, 1]$ . On one hand, the restriction to  $k, l \in \{-1, 0, 1\}$  is unnecessary. On the other hand, we shall denote  $L_j \rightarrow L_{(1)}(h_j)$  and  $N_j^{(\gamma)} \rightarrow N^{(\gamma)}(h_j)$ . [The subscript (1) indicates that only nearest neighbors are involved in the prescription of the discrete Laplacian.] By analogy, we shall write

$$\Phi_{j+k}^{j+l} \equiv (\phi_{j+l} - \phi_{j+k})/a,$$

and consequently

$$L_{(1)}(\phi_j) \equiv \frac{\Phi_j^{j+1} + \Phi_j^{j-1}}{a},$$

and

$$N^{(\gamma)}(\phi_j) \equiv \frac{\left(\Phi_j^{j+1}\right)^2 + 2\gamma \Phi_j^{j+1} \Phi_{j-1}^j + \left(\Phi_{j-1}^j\right)^2}{2(1+\gamma)}.$$

Two main symmetries are usually ascribed to the 1D KPZ equation: Galilean invariance and the fluctuation–dissipation relation.

- The first one has been traditionally linked to the exactness (in any spatial dimensionality) of the relation  $\alpha + z = 2$  among the roughness  $\alpha$  and dynamic  $z$  exponents [22, 23], although this interpretation has been recently criticized in other nonequilibrium models [24, 25]. The roughness exponent  $\alpha$  characterizes the surface morphology in the stationary regime  $t \gg t_x$ . On the other hand, the correlation length scales as  $\xi(t) \sim t^{1/z}$  with the dynamic exponent  $z$ , and  $t_x$  is the time at which it saturates, namely  $\xi(t \gg t_x) \sim L$ . The ratio  $\beta = \alpha/z$  is called “growth exponent” and characterizes the short-time behavior of the interface.
- The second symmetry essentially tells us that in 1D, the nonlinear (KPZ) term is not operative at long times or in other words, that the long-time 1D interface is equivalent to a path of Brownian motion [3]. From a theorem by Kolgomorov, this implies that the interface is Hölder continuous with exponent strictly smaller than 1/2. For higher

dimensions, the KPZ roughness exponent  $\alpha$  decreases, implying a loss of regularity. Hence the error terms of a local numerical method (as e.g. a finite differences scheme), which are proportional to some higher-order derivative of the field, are not controlled. As a consequence, a global method such as a pseudo-spectral scheme [14–16, 36] is more adequate. Nevertheless, previous experiences found in the literature showed that finite differences schemes are still able to capture the universal features of KPZ evolution. This, together with our previous considerations, is our motivation for the present work.

In Sec. II we show that the relationship established by the Hopf–Cole transformation—between the KPZ equation and a diffusion equation with multiplicative noise [2]—poses constraints on the discretization procedure. We verify the consistency of the standard (nearest-neighbor) discretization scheme and find the form of the corresponding KPZ term for a general real-space discrete Laplacian; we also present some comments regarding the mapping of KPZ into the directed polymer problem [2]. In Sec. III we analyze the problem from the perspective of the Lyapunov functional, show in what sense known prescriptions for the KPZ term from the literature fail the test, and find the corresponding consistent prescriptions. Moreover, we propose a consistent real-space discretization scheme whose accuracy is far higher than that of schemes of similar complexity in the literature. In Sec. IV we discuss the relation with the pseudo-spectral method. In Sec. V, we show that a consistent discretization scheme does not (essentially) violate the fluctuation–dissipation relation, peculiar of 1D, and discuss the role of the Galilean invariance for the discrete representations of the KPZ equation, showing that such invariance seems not to be a necessary element to define the KPZ universality class. In Sec. VI we discuss a recently introduced variational approach for the KPZ equation [26], and show that it offers a natural framework for its consistent discretization. In Section VII we present some numerical results regarding critical exponents and the violation of Galilean invariance. Section VIII contains the conclusions and final discussions. It is worth here commenting that some preliminary results were presented in [27].

## II. THE LAPLACIAN DETERMINES THE NONLINEAR TERM

In this section we elucidate—by considering the standard, nearest-neighbor discretization prescription as a benchmark—one of two constraints to be obeyed by any spatial discretization scheme. It is very important to remark that this constraint arises due to the mapping between the KPZ and the diffusion equation (with multiplicative noise) through the Hopf–Cole transformation. Hence, for a general real-space discrete Laplacian, we state the form of its corresponding KPZ term. Even though the present analysis is performed on the KPZ equation, it is general in the sense that for sets of equations related among themselves through a local transformation there should be a consistent relation between the discrete transformed forms.

### A. The simplest case

As it is known, the diffusion equation with multiplicative noise

$$\partial_t \phi = \nu \partial_x^2 \phi + \frac{\lambda F}{2\nu} \phi + \frac{\lambda \varepsilon}{2\nu} \phi \xi, \quad (2)$$

is related to the KPZ equation [Eq. (1)] through the *Hopf–Cole transformation*

$$\phi(x, t) = \exp \left[ \frac{\lambda}{2\nu} h(x, t) \right]. \quad (3)$$

Note that this transformation is just one particular example of the *general implicit transformation* written down in Ref. [28].

The standard spatial discrete version of Eq. (2), after transforming to a co-moving reference frame  $\phi \rightarrow \phi + Ft$ , is

$$\dot{\phi}_j = \nu L_{(1)}(\phi_j) + \frac{\lambda \varepsilon}{2\nu} \phi_j \xi_j, \quad (4)$$

with  $1 \leq j \leq N \equiv 0$ , because periodic boundary conditions are assumed as usual (the implicit sum convention is not meant in any of the discrete expressions). The discrete noise  $\xi_j(t)$  is a Gaussian random variable with zero mean and correlation given by

$$\langle \xi_j(t) \xi_k(t') \rangle = 2 \frac{\delta_{jk}}{a} \delta(t - t'). \quad (5)$$

Then, using the discrete version of Eq. (3)

$$\phi_j(t) = \exp \left[ \frac{\lambda}{2\nu} h_j(t) \right], \quad (6)$$

we get

$$e^{\frac{\lambda}{2\nu}h_j} \frac{\lambda}{2\nu} \dot{h}_j = \frac{\nu}{a^2} L_{(1)} \left( e^{\frac{\lambda}{2\nu}h_j} \right) + \frac{\lambda\varepsilon}{2\nu} e^{\frac{\lambda}{2\nu}h_j} \xi_j,$$

namely

$$\dot{h}_j = \frac{2\nu^2}{\lambda a^2} \left[ e^{\delta_j^+ a} + e^{\delta_j^- a} - 2 \right] + \varepsilon \xi_j,$$

with  $\delta_j^\pm \equiv \frac{\lambda}{2\nu} H_j^{j\pm 1}$ . It is worth commenting here that this last expression was also pointed out in [9], discussing aspects of discretization instabilities and the relation to the directed polymer problem. We will further discuss the mapping to the directed polymer problem in Sec. II C below. By expanding the exponentials up to terms of order of  $a^2$ , and collecting equal powers of  $a$  (observe that the zero-order contribution vanishes) we retrieve

$$\dot{h}_j = \nu L_{(1)}(h_j) + \frac{\lambda}{2} Q_{(1)}(h_j) + \varepsilon \xi_j, \quad (7)$$

with

$$Q_{(1)}(h_j) = \frac{1}{2} \left[ \left( H_j^{j+1} \right)^2 + \left( H_j^{j-1} \right)^2 \right], \quad (8)$$

( $Q$  stands for “quadratic”). As we see, the first and second terms on the r.h.s. of Eq. (7) are *necessarily* related by virtue of Eq. (6).

## B. The general case

A Taylor expansion of  $\phi_{j+l}$  around  $\phi_j$  shows that the general form of the discrete Laplacian, involving up to the  $n$ -th nearest neighbors of site  $j$ , is of the form

$$L_{(n)}(\phi_j) = \frac{\sum_{l=1}^n b_l \left[ \Phi_j^{j+l} + \Phi_j^{j-l} \right]}{a \sum_{l=1}^n l^2 b_l}, \quad (9)$$

where as before, the subscript stands for the number of nearest neighbors. Since the maximum value for  $n$  is  $M \equiv (N-1) \setminus 2$ , where  $\setminus$  denotes integer division, one may alternatively run the sum up to  $M$  and set  $b_l = 0$ ,  $l = n+1 \dots M$ . The remaining  $b_l$ , that are otherwise arbitrary, should be fixed by whatever criterion (below, we shall use the criterion of maximizing accuracy).

Repeating the steps described above, one obtains

$$L_{(n)}(h_j) = \frac{\sum_{l=1}^n b_l \left[ H_j^{j+l} + H_j^{j-l} \right]}{a \sum_{l=1}^n l^2 b_l}, \quad (10)$$

$$Q_{(n)}(h_j) = \frac{\sum_{l=1}^n b_l \left[ \left( H_j^{j+l} \right)^2 + \left( H_j^{j-l} \right)^2 \right]}{2 \sum_{l=1}^n l^2 b_l}. \quad (11)$$

### C. Few remarks on the directed polymer problem

We devote this subsection to briefly comment about the mapping of KPZ onto the directed polymer problem. Such a mapping can be carried out via the Hopf-Cole transformation [9] and the resulting linear equation corresponds to Eq. (2). In order to employ the usual rules of calculus, here we assume the Stratonovich interpretation for the multiplicative noise. The corresponding finite differences scheme is, explicitly,

$$\dot{\phi}_j = \nu L_{(1)}(\phi_j) + \frac{\lambda F}{2\nu} \phi_j + \frac{\lambda \varepsilon}{2\nu} \phi_j \xi_j(t). \quad (12)$$

As indicated in Eq. (5), the discrete noise  $\xi_j(t)$  is a Gaussian random variable. The mean value of Eq. (12) is

$$\frac{d\langle\phi_j\rangle}{dt} = \nu \frac{\langle\phi_{j+1}\rangle + \langle\phi_{j-1}\rangle - 2\langle\phi_j\rangle}{a^2} + \frac{\lambda F}{2\nu} \langle\phi_j\rangle + \frac{\lambda \varepsilon}{4\nu a} \langle\phi_j\rangle. \quad (13)$$

One immediately realizes that the drift of this equation becomes singular in the continuum limit  $a \rightarrow 0$ , so one has to renormalize this theory [29–31]. This is done by decomposing the bare parameter into an effective and a singular component,  $F = F_{\text{eff}} + F_s$ , with  $F_s = -1/(2a)$ . The resulting equation is then

$$\frac{d\langle\phi_j\rangle}{dt} = \nu \frac{\langle\phi_{j+1}\rangle + \langle\phi_{j-1}\rangle - 2\langle\phi_j\rangle}{a^2} + \frac{\lambda F_{\text{eff}}}{2\nu} \langle\phi_j\rangle, \quad (14)$$

which is finite, but in which  $F_{\text{eff}}$  has to be measured directly from the experiment. Thus the correct interpretation of the Stratonovich Eq. (12) is the following Itô equation

$$\dot{\phi}_j = \nu \frac{\phi_{j+1} + \phi_{j-1} - 2\phi_j}{a^2} + \frac{\lambda F_{\text{eff}}}{2\nu} \phi_j + \frac{\lambda \varepsilon}{2\nu} \phi_j \xi_j(t). \quad (15)$$

In order to measure the effective growth rate, one can solve the linear Eq. (14) to find the globally stable solution  $\langle\phi_j(t)\rangle = \langle\phi_j(0)\rangle \exp[\lambda F_{\text{eff}} t/(2\nu)]$  for a spatially homogeneous initial condition  $\langle\phi_j(0)\rangle = \langle\phi(0)\rangle$ . And so this effective rate can be measured from experimental/numerical data in the following fashion

$$F_{\text{eff}} = \frac{2\nu}{\lambda t} \ln[\langle\phi_j(t)\rangle/\langle\phi_j(0)\rangle], \quad (16)$$

or alternatively

$$F_{\text{eff}} = \frac{2\nu}{\lambda t} \ln \{ \langle \exp[\lambda h_j(t)/(2\nu)] \rangle \}, \quad (17)$$

assuming that the initial condition is  $h_j(0) = 0$ . Applying Jensen's inequality to this last relation one finds

$$\langle h_j(t) \rangle \geq F_{\text{eff}} t, \quad (18)$$

in agreement with what one could directly obtain from the KPZ equation [Eq. (1)].

### III. EXPLOITING THE DETERMINISTIC LYAPUNOV FUNCTIONAL

An important feature of the Hopf–Cole transformation—Eq. (3) or (6)—is that it is *local*, i.e. it involves neither spatial nor temporal transformations. Some effects of this feature are the following

1. The discrete form of the Laplacian—namely the operator  $L_{(n)}$ —is the same, regardless of whether it is applied to  $\phi$  or to  $h$ .
2. For a given  $L_{(n)}$  (i.e. a given set of  $b_l = 0$ ,  $l = 1 \dots n$ ),  $Q_{(n)}$  is *determined* by the Hopf–Cole transformation, Eq. (6).

In this section, we want to go further with the criterion that the definitions of the discrete operators should not depend on the fields on which they are applied.

The *deterministic* part of Eq. (2), namely the diffusion term, admits a local Lyapunov functional. In other words, for  $\varepsilon = 0$ , Eq. (2) can be written in the following variational form

$$\partial_t \phi = -\frac{\delta \mathcal{F}[\phi]}{\delta \phi}, \quad (19)$$

with

$$\mathcal{F}[\phi] = \frac{\nu}{2} \int dx (\partial_x \phi)^2. \quad (20)$$

The aforementioned criterion dictates the following set of discrete forms (thus Lyapunov functions, for any finite  $N$ ) of Eq. (20)

$$\mathcal{F}_{(n)}[\phi] = \frac{1}{2} \nu a \sum_{j=1}^N Q_{(n)}(\phi_j). \quad (21)$$

It is a trivial task to verify that

$$\nu L_{(n)}(\phi_j) = -\frac{1}{a} \frac{\partial \mathcal{F}_{(n)}[\phi]}{\partial \phi_j}. \quad (22)$$



There is no loss of generality in taking  $j = N \equiv 0$ . If we rearrange the sum in Eq. (21) as  $\sum_{j=M+1-N}^M$ , with  $M \equiv (N-1)\backslash 2$ , then only  $-n \leq j \leq n$  will contribute in Eq. (22). Moreover, their contribution is such that they cancel the factor  $1/2$  in front of the sum in Eq. (21). For completeness, let us show the particular functional form for  $Q_{(1)}(\phi_j)$

$$\mathcal{F}_{(1)}[\phi] = \frac{\nu}{4a} \sum_{j=1}^N [(\phi_{j+1} - \phi_j)^2 + (\phi_j - \phi_{j-1})^2]. \quad (23)$$

### A. Other discrete forms of the KPZ term

Of course, Eq. (22) does not *uniquely* determine the Lyapunov function. Expressions other than Eq. (21) may yield  $L_{(n)}(\phi_j)$ , provided that they contain the right terms, in the right proportion. Take as an example the proposal of Refs. [10, 11], coded as  $N_j^{(1/2)}$  in Ref. [19]

$$N^{(1/2)}(\phi_j) = \frac{1}{3} \left[ (\Phi_j^{j+1})^2 + (\Phi_j^{j-1})^2 - \Phi_j^{j+1} \Phi_j^{j-1} \right]. \quad (24)$$

By using  $N^{(1/2)}(\phi_{j'})$  instead of  $Q_{(n)}(\phi_{j'})$  in Eq. (20), we obtain

$$\begin{aligned} L_{(2)}^{(1/2)}(\phi_j) &\equiv \frac{1}{6} \left[ 2(\Phi_j^{j+1} + \Phi_j^{j-1}) + (\Phi_j^{j+2} + \Phi_j^{j-2}) \right] \\ &= \frac{1}{6} \left[ 2L_{(1)}(\phi_j) + \frac{1}{a} (\Phi_j^{j+2} + \Phi_j^{j-2}) \right], \end{aligned} \quad (25)$$

which is an instance of  $L_{(2)}(\phi_j)$ , with  $b_1 = 2$ ,  $b_2 = 1$ . As it was shown before, the procedure outlined in Sec. II will yield  $L_{(2)}^{(1/2)}(h_j)$ , together with

$$Q_{(2)}^{(1/2)}(h_j) \equiv \frac{1}{12} \left\{ 2 \left[ (H_j^{j+1})^2 + (H_j^{j-1})^2 \right] + \left[ (H_j^{j+2})^2 + (H_j^{j-2})^2 \right] \right\} \quad (26)$$

and *not*  $N^{(1/2)}(h_j)$ . Hence, the proposal of Refs. [10, 11] is not consistent: On one hand,  $N^{(1/2)}(h_j)$  does not correspond with  $L_{(1)}(h_j)$ , as it is used. On the other hand, it does not correspond with  $L_{(2)}^{(1/2)}(h_j)$  either, as shown.

As stated before, the proposal of Refs. [10, 11] belongs to a family coded in Ref. [19] as  $N_j^{(\gamma)}$ ,  $\gamma \in [0, 1]$ . The choice  $\gamma = 1$  yields  $N^{(1)}(\phi_j) = \frac{1}{4} (\Phi_{j-1}^{j+1})^2$ . On the other hand, the choice  $\gamma = 0$  yields  $L_{(2)}^{(0)}(h_j) = L_{(1)}(h_j)$ . They all correspond to  $n = 2$ , with  $b_1 = 1 - \gamma$ ,  $b_2 = \gamma/2$ . The equivalent of Eq. (24) is now

$$N^{(\gamma)}(\phi_j) = \frac{1}{2(1+\gamma)a^2} \left[ (\Phi_j^{j+1})^2 + (\Phi_j^{j-1})^2 - 2\gamma \Phi_j^{j+1} \Phi_j^{j-1} \right], \quad (27)$$

which  $\forall \gamma \in [0, 1]$  yields

$$\begin{aligned} L_{(2)}^{(\gamma)}(h_j) &\equiv \frac{1}{1+\gamma} \left[ (1-\gamma) (H_j^{j+1} + H_j^{j-1}) + \frac{\gamma}{2} (H_j^{j+2} + H_j^{j-2}) \right] \\ &= \frac{1}{2(1+\gamma)} \left\{ 2L_{(1)}(h_j) + \gamma [L_{(1)}(h_{j+1}) + L_{(1)}(h_{j-1})] \right\} \end{aligned} \quad (28)$$

and

$$Q_{(2)}^{(\gamma)}(h_j) \equiv \frac{1}{2(1+\gamma)} \left\{ (1-\gamma) [(H_j^{j+1})^2 + (H_j^{j-1})^2] + \frac{\gamma}{2} [(H_j^{j+2})^2 + (H_j^{j-2})^2] \right\}. \quad (29)$$

However, the accuracy of this discretization is unknown and should be studied.

## B. A more accurate discretization scheme

Again, a Taylor expansion of  $\phi_{j+l}$  around  $\phi_j$  shows that the  $\mathcal{O}(a^2)$  corrections to  $L_{(n)}$  [applied to  $h_j$  in Eq. (10)] are of the form

$$\frac{2}{4!} \frac{\sum_{l=1}^n l^4 b_l}{\sum_{l=1}^n l^2 b_l} \partial_x^4 h.$$

Thus, the  $\mathcal{O}(a^2)$  correction to  $L_{(2)}^{(\gamma)}$  is  $\frac{1}{12} \frac{1+7\gamma}{1+\gamma} \partial_x^4 h$ . It attains its minimum value ( $\frac{1}{12} \partial_x^4 h$ ) precisely for  $\gamma = 0$ , namely for  $L_{(1)}$ . What is then the convenience of a more complex prescription for the Laplacian?

A wise criterion for choosing  $b_1$  and  $b_2$  in  $L_{(2)}$  is making the  $\mathcal{O}(a^2)$  corrections vanish. This yields the prescription  $b_1 = 16$ ,  $b_2 = -1$ , known to be accurate up to corrections of  $\mathcal{O}(a^4)$  [32].

Carrying out the procedure sketched in Sec. II A, we obtain

$$L_{(2)}(h_j) \equiv \frac{4}{3} L_{(1)}(h_j) - \frac{1}{12} (H_j^{j+2} + H_j^{j-2}), \quad (30)$$

$$Q_{(2)}(h_j) \equiv \frac{2}{3} [(H_j^{j+1})^2 + (H_j^{j-1})^2] - \frac{1}{24} [(H_j^{j+2})^2 + (H_j^{j-2})^2]. \quad (31)$$

The  $\mathcal{O}(a^2)$  corrections to  $Q_{(n)}$  are

$$\frac{2}{4!} \frac{\sum_{l=1}^n l^4 b_l}{\sum_{l=1}^n l^2 b_l} \left[ 3 (\partial_x^2 h)^2 + 4 (\partial_x^3 h) (\partial_x h) \right],$$

which also vanishes for  $b_1 = 16$ ,  $b_2 = -1$ .

Since this discretization scheme fulfills the consistency conditions, is accurate up to  $\mathcal{O}(a^4)$  corrections, and its prescription is not more complex than the ones studied before, it is

obvious that it will be a convenient one to be used when a higher accuracy in numerical schemes is required. The possibility that it may also help to control (or at least delay) the numerical instabilities found in previous works (see for instance [9, 33] and references therein) will be the subject of further work.

Let us remind again that, as we already pointed out in the introduction, these results are formal since the higher order derivatives of the field are not under control.

#### IV. PSEUDO-SPECTRAL DISCRETIZATION

As was indicated in the introduction, a pseudo-spectral spatial discretization scheme has been recently introduced [14–16, 36]. In this section we show the relation existing between the present analysis and the indicated pseudo-spectral spatial discretization scheme.

The pseudo-spectral discretization procedure starts by Fourier expanding the field  $h(x, t)$

$$h(x, t) = \sum_{k=-\infty}^{\infty} \hat{h}_k(t) \exp\left(i\frac{2\pi}{L}kx\right), \quad (32)$$

with

$$\hat{h}_k(t) = \frac{1}{L} \int_0^L dx h(x, t) \exp\left(-i\frac{2\pi}{L}kx\right), \quad (33)$$

and Eq. (3) can be rewritten as

$$\phi(x, t) = \exp\left[\frac{\lambda}{2\nu} \sum_{k=-\infty}^{\infty} \hat{h}_k(t) \exp\left(i\frac{2\pi}{L}kx\right)\right]. \quad (34)$$

Thus Eq. (2) reads

$$\sum_{k=-\infty}^{\infty} \exp\left(i\frac{2\pi}{L}kx\right) \left\{ \dot{\hat{h}}_k(t) + \left(\frac{2\pi}{L}\right)^2 k \hat{h}_k(t) \left[ \nu k + \frac{\lambda}{2} \sum_{k'=-\infty}^{\infty} k' \hat{h}_{k'}(t) \exp\left(i\frac{2\pi}{L}k'x\right) \right] - \varepsilon \hat{\xi}_k(t) \right\} = 0, \quad (35)$$

since  $\xi(x, t)$  is also assumed to be  $L$ -periodic as a function of  $x$ . A *sufficient* condition is that

$$\dot{\hat{h}}_k(t) = -\left(\frac{2\pi}{L}\right)^2 k \hat{h}_k(t) \left[ \nu k + \frac{\lambda}{2} \sum_{k'=-\infty}^{\infty} k' \hat{h}_{k'}(t) \exp\left(i\frac{2\pi}{L}k'x\right) \right] + \varepsilon \hat{\xi}_k(t). \quad (36)$$

In this context “discretize” means to consider only  $N$  Fourier modes, including  $k = 0$ . If  $M \equiv (N - 1) \setminus 2$ , then

$$\dot{\hat{h}}_k(t) = -\left(\frac{2\pi}{L}\right)^2 k \hat{h}_k(t) \left[ \nu k + \frac{\lambda}{2} \sum_{k'=M+1-N}^M k' \hat{h}_{k'}(t) \exp\left(i\frac{2\pi}{L}k'x\right) \right] + \varepsilon \hat{\xi}_k(t). \quad (37)$$

As indicated before, it is interesting to connect real-space and pseudo-spectral discretization approaches. From Eq. (32) [with  $h(ja, t) \equiv h_j(t)$ ] we have

$$H_j^{j+l} = \frac{2}{a} \sum_{k=M+1-N}^M \hat{h}_k(t) \sin\left(\frac{\pi kl}{N}\right) \exp\left[i\frac{2\pi}{N}k\left(j + \frac{l}{2}\right)\right], \quad (38)$$

and

$$L_{(M)}(h_j) = \sum_{k=M+1-N}^M \hat{h}_k(t) \left\{ \frac{2a \sum_{l=1}^M b_l \left[ \cos\left(\frac{2\pi kl}{N}\right) - 1 \right]}{a \sum_{l=1}^M l^2 b_l} \right\} \exp\left(i\frac{2\pi}{N}kj\right) \quad (39)$$

By equating this expression to

$$- \sum_{k=M+1-N}^M \hat{h}_k(t) \left(\frac{2\pi k}{L}\right)^2 \exp\left(i\frac{2\pi}{N}kj\right),$$

we might think of the pseudo-spectral discretization as a particular real-space discretization, whose coefficients are the solutions of the linear system

$$\sum_{l=1}^M b_l \left[ \cos\left(\frac{2\pi kl}{N}\right) - 1 + \frac{1}{2} \left(\frac{2\pi kl}{N}\right)^2 \right] = 0. \quad (40)$$

This equation is linear and homogeneous, and so it admits the trivial solution  $b_l = 0 \forall l \in \{1, \dots, M\}$ . This equation expresses in fact the fundamental difference of the spectral and finite differences discretization: the lattice spectrum. For the finite difference scheme the discrete Laplacian is no longer  $(2\pi k/L)^2$  (namely twice the spectrum in the continuum) but  $1 - \cos\frac{2\pi kx}{L}$ . For  $x = L/2$ , already for  $k = 1$  the difference is  $\pi^2/2 - 2 \approx 3$ . If we equate instead Eq. (39) to

$$\sum_{k=M+1-N}^M \hat{h}_k(t) \left[ \cos\left(\frac{2\pi kl}{N}\right) - 1 \right] \exp\left(i\frac{2\pi}{N}kj\right),$$

then Eq. (40) says nothing new. There is still a complete arbitrariness in the choice of the coefficients  $b_l$ . This corresponds to the fact that this scheme is nothing but the Fourier transformed version of the finite differences one.

## V. GALILEAN INVARIANCE AND FLUCTUATION-DISSIPATION RELATION

There are two main symmetries associated with the 1D KPZ equation: the fluctuation-dissipation relation and Galilean invariance. On one hand the fluctuation-dissipation relation essentially tells us that the nonlinearity is asymptotically (that is, at long times) not operative in 1D. On the other hand, Galilean invariance has been traditionally related to the exact relation among exponents  $\alpha + z = 2$ , that holds for all spatial dimensions [22, 23]. However, it is worth remarking that this interpretation has been recently criticized [24].

### A. Galilean Invariance

Galilean invariance means that the KPZ equation is invariant under the transformation

$$\begin{aligned} x &\rightarrow x - \lambda v t, \\ h &\rightarrow h + v x, \\ F &\rightarrow F - \frac{\lambda}{2} v^2, \end{aligned} \tag{41}$$

where  $v$  is an arbitrary constant vector field and  $F$  is the external (constant) driving force. Using the classical discretization

$$\partial_x h \rightarrow \frac{1}{2} H_{j-1}^{j+1}, \tag{42}$$

for the (complete) KPZ equation, we find

$$\dot{h}_j = \nu L_1 + \frac{\lambda}{8} \left( H_{j-1}^{j+1} \right)^2 + F + \xi_j(t). \tag{43}$$

One can immediately check that this equation is invariant under the *discrete* Galilean transformation

$$\begin{aligned} j a &\rightarrow j a - \lambda v t, \\ h_j &\rightarrow h_j + v j a, \\ F &\rightarrow F - \frac{\lambda}{2} v^2. \end{aligned} \tag{44}$$

However, Eq. (43) has been criticized for its instability properties, at least when the spatial discretization is not fine enough [9]. If we use the alternative discretization

$$\dot{h}_j = \nu L_1(h_j) + \frac{\lambda}{4} \left[ \left( H_j^{j+1} \right)^2 + \left( H_{j-1}^j \right)^2 \right] + F + \xi_j(t), \tag{45}$$

we find that this equation is *not* invariant under the discrete Galilean transformation. In fact, the transformation  $h \rightarrow h + v j a$  yields an excess term which is compatible with the gradient discretization in Eq. (42); however, this discretization does not allow to recover the quadratic term in Eq. (45), indicating that this finite differences scheme does not fulfill Galilean invariance. The Hopf–Cole transformed equation

$$\dot{\phi}_j = \nu L_j(\phi) + \frac{\lambda F}{2\nu} \phi_j + \frac{\lambda}{2\nu} \phi_j \xi_j(t), \tag{46}$$

is Galilean invariant, i.e., it is invariant under the transformation indicated in Eqs. (44). Hence, the nonlinear Hopf-Cole transformation is responsible for the loss of Galilean invariance. Note that these results are independent of whether we consider this discretization scheme or a more accurate one.

Galilean invariance has been always associated with the exactness of the 1D KPZ exponents, and with a relation that connects the critical exponents in higher dimensions. If the numerical solution obtained from a finite differences scheme as Eq. (45), which is not Galilean invariant, *yields the well known critical exponents*, that would strongly suggest that Galilean invariance is not a fundamental symmetry as usually considered.

In Sec. VII we present some numerical results for the critical exponents using the consistent discretization schemes indicated in Eqs. (8) and (31), and compare with those found with the standard one. All the cases exhibit the same critical exponents. Moreover, let us note that the discretization used in Refs. [10, 11], which also violates Galilean invariance, yields the same critical exponents too.

When we compare the classical discretization given by Eq. (43), that explicitly reads

$$\dot{h}_j = \nu \frac{h_{j+1} + h_{j-1} - 2h_j}{a^2} + \frac{\lambda}{2} \left( \frac{h_{j+1} - h_{j-1}}{2a} \right)^2 + F + \xi_j(t). \quad (47)$$

with the alternative one in Eq. (45), that reads

$$\dot{h}_j = \nu \frac{h_{j+1} + h_{j-1} - 2h_j}{a^2} + \frac{\lambda}{4} \left[ \left( \frac{h_{j+1} - h_j}{a} \right)^2 + \left( \frac{h_j - h_{j-1}}{a} \right)^2 \right] + F + \xi_j(t), \quad (48)$$

we find that this second one presents excess fluctuations with respect to the first. This can be easily seen by means of the inequality

$$(h_{j+1} - h_{j-1})^2 = (h_{j+1} - h_j + h_j - h_{j-1})^2 \leq 2(h_{j+1} - h_j)^2 + 2(h_j - h_{j-1})^2, \quad (49)$$

which immediately translates into

$$\frac{\lambda}{2} \left( \frac{h_{j+1} - h_{j-1}}{2a} \right)^2 \leq \frac{\lambda}{4} \left[ \left( \frac{h_{j+1} - h_j}{a} \right)^2 + \left( \frac{h_j - h_{j-1}}{a} \right)^2 \right], \quad (50)$$

where the inequality is strict unless  $h_j = (h_{j+1} + h_{j-1})/2$ , an event which happens with zero probability (note that in 1D and for long times, the KPZ interface has independent Gaussian distributed increments, as Brownian motion). This implies that the excess fluctuations are genuinely present in the interface dynamics.

The excess fluctuations from Eq. (48) respect to Eq. (47) can be explicitly computed: the alternative discretization scheme may be written as

$$\begin{aligned} \dot{h}_j = & \nu \frac{h_{j+1} + h_{j-1} - 2h_j}{a^2} + \frac{\lambda}{2} \left\{ \frac{h_{j+1} - h_{j-1}}{2a} \right\}^2 + \\ & + \frac{\lambda}{4a^2} \left[ \frac{1}{2}h_{j+1}^2 + \frac{1}{2}h_{j-1}^2 + 2h_j^2 - 2h_{j+1}h_j - 2h_jh_{j-1} + h_{j+1}h_{j-1} \right] \\ & + F + \xi_j(t), \end{aligned} \quad (51)$$

where the term between curly brackets denotes the Galilean invariant fluctuations and the term between square brackets denotes the excess fluctuations. If the excess fluctuations are comparable to the Galilean fluctuations then there will be a strong violation of Galilean invariance. If the critical exponents still persist in this case, that would indicate that Galilean invariance is not such a fundamental symmetry as usually considered. This will be discussed in Sec. VII.

### B. Fluctuation–dissipation relation: stationary probability distribution

As we have already mentioned, together with Galilean invariance, the fluctuation–dissipation relation is another fundamental symmetry of the 1D KPZ equation. It is clear that both these symmetries are recovered when taking the continuum limit on any reasonable discretization scheme. And thus, an accurate enough partition must yield suitable results.

The stationary probability distribution for the KPZ problem in 1D is known to be [2, 3]

$$\mathcal{P}_{\text{stat}}[h] \sim \exp \left\{ \frac{\nu}{2\varepsilon} \int dx (\partial_x h)^2 \right\}.$$

For the simplest discretization scheme in Eq. (22), we have

$$\mathcal{P}_{\text{stat}}[h] \sim \exp \left\{ \frac{\nu}{2\varepsilon} \sum_j \frac{1}{2} \left[ (H_j^{j+1})^2 + (H_j^{j-1})^2 \right] \right\}. \quad (52)$$

Inserting this expression into the stationary Fokker–Planck equation several terms cancel, and the ones surviving can be expressed as

$$\lambda\nu \sum_j \frac{1}{2} \left[ (H_j^{j+1})^2 + (H_j^{j-1})^2 \right] L_j^{(0)}. \quad (53)$$

Clearly, the continuous limit of this expression is of the form

$$\lambda\nu \int dx (\partial_x h)^2 \partial_x^2 h,$$

that, as is well known [2], is identically zero. A numerical analysis of Eq. (53) indicates that this expression is several orders of magnitude smaller than the value of the pdf's exponent [Eq. (52)], and typically behaves as  $\mathcal{O}(1/N)$ , where  $N$  is the number of spatial points used in the discretization. Moreover, using expressions with higher accuracy for the differential operators one gets an even faster approach to zero. This indicates that the problem with the fluctuation–dissipation theorem in  $1+1$ , discussed in [11, 15] can be just circumvented using more accurate expressions. It is also worth commenting that, if a consistent discrete scheme is built from the discrete scheme in [11], it would also violate the fluctuation–dissipation relation.

## VI. ON THE VARIATIONAL FORMULATION OF KPZ

In Ref. [26], a variational formulation was introduced for the KPZ equation. There it was shown that Eq. (1) can be written as

$$\partial_t h(x, t) = -\Gamma(h) \frac{\delta \mathcal{G}[h]}{\delta h(x, t)} + \varepsilon \xi(x, t); \quad (54)$$

where (for  $F = 0$ )

$$\mathcal{G}[h] = \int_{\Omega} e^{\frac{\lambda}{\nu} h(x, t)} \frac{\lambda^2}{8\nu} [\partial_x h(x, t)]^2 dx, \quad (55)$$

and the function  $\Gamma(h)$  is given by

$$\Gamma(h) = \left( \frac{2\nu}{\lambda} \right)^2 e^{-\frac{\lambda}{\nu} h}.$$

The way in which the functionals  $\mathcal{F}[\phi]$  and  $\mathcal{G}[h]$  are related is also shown in Ref. [26]. It is also easy to prove that the functional  $\mathcal{G}[h]$  fulfills the Lyapunov property  $\partial_t \mathcal{G}[h] \leq 0$ .

According to the previous results, we can write the discrete version of Eq. (55) as

$$\mathcal{G}[h] = \frac{\lambda^2}{8\nu} \sum_j e^{\frac{\lambda}{\nu} h_j} \frac{1}{2} [(H_j^{j+1})^2 + (H_j^{j-1})^2].$$

Now, introducing this expression into the discrete version of Eq. (54), and through a simple algebra, we reobtain Eq. (7). This reinforces our result, and clearly indicates the need to be consistent when considering a discrete version of the KPZ equation.



## VII. SOME NUMERICAL RESULTS

We present here some results obtained by numerically integrating the KPZ equation in 1D. Our aim is to compare the standard discretization scheme [Eq. (47)] with the consistent ones presented in Eqs. (10) and (53).

To solve Eq. (1) we discretize  $h(x, t)$  along the substrate direction  $x$  with lattice spacing  $a = 1$ . We employ a second-order Runge–Kutta algorithm (see e.g. [34]) with periodic boundary conditions. Then the equation of motion

$$\dot{h}_j = \nu L(h_j) + \frac{\lambda}{2} Q(h_j) + \varepsilon \xi_j = F(h_j) + \varepsilon \xi_j \quad (56)$$

is integrated according to the recursive relation

$$h_j(t + \Delta t) = h_j + \frac{\Delta t}{2}(g_1 + g_2) + (\Delta t)^{1/2} u_j, \quad (57)$$

with

$$\begin{aligned} g_1 &= F(h_j) \\ g_2 &= F(h_j + \Delta t g_1 + (\Delta t)^{1/2} u_j), \end{aligned}$$

where  $u_j$  is a Gaussian random variable.

Without loss of generality, the interface dynamics can be described in terms of the dimensionless parameter  $\tilde{\lambda} = (2\varepsilon/\nu^3)^{1/2}\lambda$ . In practice, we set  $\nu = \varepsilon = 1$  and allow  $\lambda$  to vary.

The numerical results show that the interface scaling does not depend on the discretization scheme. As shown in Fig. 1, the dynamics fit into the KPZ universality class for all the discretization schemes. The global width, that concerns the fluctuations of the growth height around its mean value, scales according to the Family–Vicsek Ansatz [3] as

$$W(L, t) = t^\beta f(t/t_x) = t^\beta f(t/L^z), \quad (58)$$

where the scaling function  $f(u)$  is defined as

$$f(u) \sim \begin{cases} \text{const} & \text{if } u \ll 1, \\ u^{-\beta} & \text{otherwise.} \end{cases} \quad (59)$$

On the other hand, correlations can be analyzed in the reciprocal space by means of the structure factor

$$S_k(t) = \langle \hat{h}_k(t) \hat{h}_{-k}(t) \rangle, \quad (60)$$

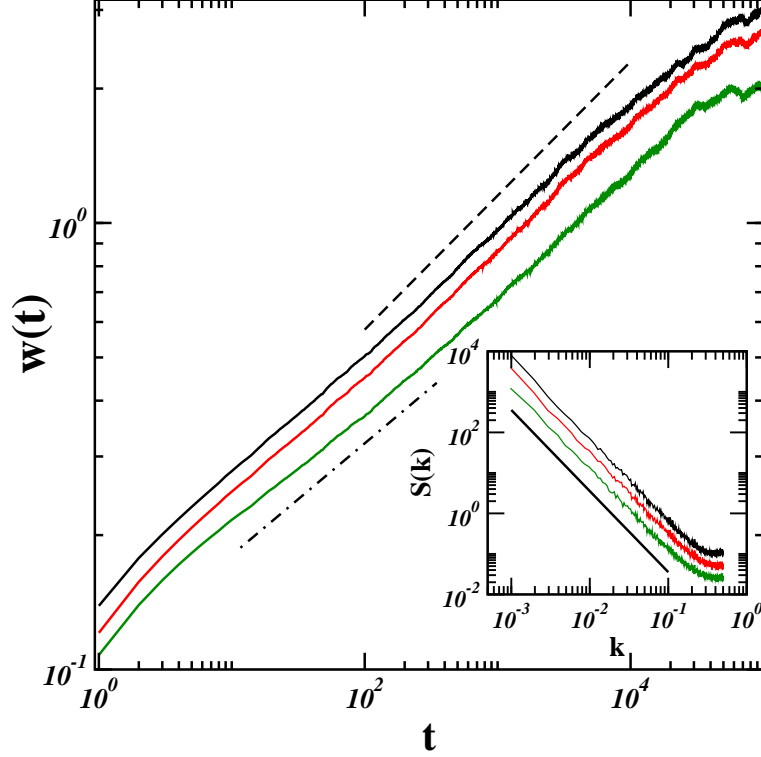


FIG. 1: Numerical results for the global width and structure factor (*inset*) averaged over 100 runs in a system of size  $L = 1024$  with  $\lambda = 4$ . We employ the different discretization schemes indicated in Eqs. (47), (48) and (30,31) (from bottom to top). Curves are slightly shifted vertically for clarity. Lines are plotted as a guide with exponent  $\beta_{\text{KPZ}} = 0.3$  (*dashed*),  $\beta = 0.25$  (*dot-dashed*), and  $-2$  (*solid, in the inset*). All discretization schemes are consistent with the KPZ scaling.

where  $\hat{h}_k(t)$  is as before (see Sec. IV) the Fourier transform of the interface profile. According to the previous scaling Ansatz,  $S(k, t)$  scales as  $k^{-(2\alpha+1)}$  with the roughness exponent  $\alpha$ .

We observe that all the discretization schemes are consistent with the KPZ scaling, with the KPZ exponents  $\alpha = 1/2$  and  $\beta = 1/3$ . It can also be observed from Fig. 1 that the crossover from the transient linear (Edwards–Wilkinson) behavior to the asymptotic nonlinear (KPZ) behavior appears earlier in both alternative discretization schemes than in the standard one [Eq. (47)]. This effect is presumably related to the fact that the nonlinearity of the alternative schemes always makes a much stronger contribution to the dynamics than the one in the standard scheme, see Fig. 2 below. This way, the threshold contribution from the nonlinearity is received sooner, resulting in an anticipated departure from the transient linear regime.

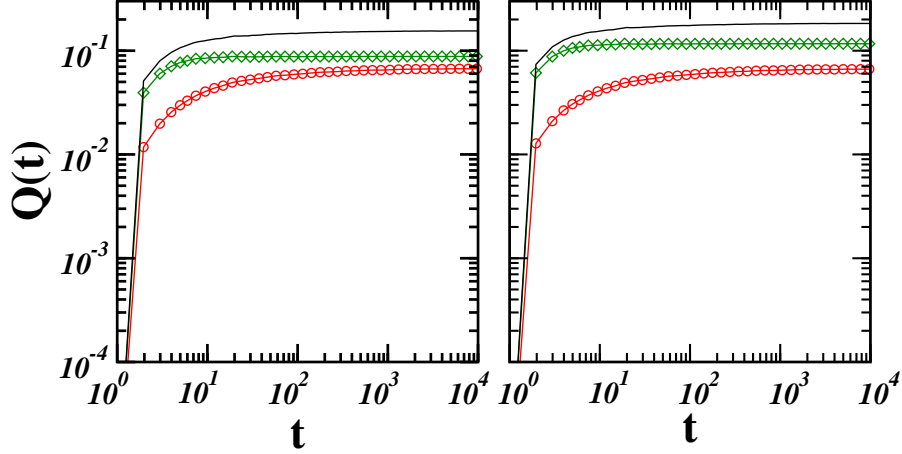


FIG. 2: Solid line: Time dependence of the nonlinear contribution in two discretization schemes [Eq. (10) (left frame) and Eq. (53) (right frame)]. We also depict the Galilean contribution (circles) and the excess of fluctuations (diamonds) as defined e.g. in Eq. (51). For both cases, the excess of fluctuations are comparable with the Galilean contribution.

In order to analyze the excess of fluctuations that such discretization schemes present with respect to the standard one, we extract the Galilean invariant fluctuations from the quadratic term of the equation of motion. In Fig. 2 we depict the time dependence of the different nonlinear contributions for both alternative discretization schemes. On the left we have the comparison between the discretization scheme Eq. (47) and the one in Eq. (48), while on the right we compare the scheme in Eq. (47) to the one in Eqs. (30,31).

The first point to note is the rapid saturation of nonlinearities. This behavior is consistent with the rapid saturation of local fluctuations, which behave as  $G(\ell, t) \sim t^{2\beta}$  and saturate for  $t \gg \ell^z$  [35]. We also observe that for both cases, the excess of fluctuations are comparable to (or even larger than) the Galilean contribution. As we pointed out in previous sections, this result, together with the persistence of KPZ scaling shown in Fig. 1, would imply that Galilean invariance is not such a fundamental symmetry as usually considered. It is worth remarking that the present results are not affected by either changing  $L$  or using other algorithms [21] to perform the numerical simulations.

## VIII. CONCLUSIONS

The moral from the present analysis is clear: due to the constraint imposed by the Hopf–Cole transformation [Eqs. (3) and (6)] the discrete forms of the Laplacian and the nonlinear KPZ term cannot be chosen independently.

Although the present work is focused on the relation between the diffusion equation with multiplicative noise and the KPZ equation, the consequences of this analysis are more general. The discrete versions of any set of related differential equations should be obtained taking into account the original (or leading) equation and the transformation rules. It is worth remarking here that a related analysis was done in [9], but there the emphasis was on the study of the strong coupling limit and the mapping onto the directed polymer problem, without commenting at all about the consistency among the discrete versions of the differential operators.

The results discussed here are general; they neither depend on space dimensionality nor rely on variational representations. Nonetheless, the recently introduced variational approach for KPZ [26] offers an adequate framework in order to make a consistent discretization of the KPZ equation.

Regarding the recently introduced pseudo-spectral approach [14, 16, 36], in addition to its known advantages, in principle, it seems to have the virtue of being “transparent” respect to the present problem. In this respect, we have shown the relation that exists between it and the present analysis. Besides that, when analyzing inhomogeneous situations where defects or impurities are present, such methods do not apply and it is again necessary to resort to real-space discrete form of the differential operators [21, 37]. Another aspect to consider is related to the situation in [33], where a problem of numerical instabilities (a computational problem) in discrete growth models has been tackled by introducing higher order contributions (changing the physics of the problem!). It is worth indicating that such an instability does not seem to arise (or at least it arises latter) in pseudo-spectral treatments of the same problem. Hence, due to the relation among both formalisms, it seems reasonable to expect that such instabilities could at least be delayed if a consistent discretization scheme, together with higher order discrete operators, is used.

Regarding the two main symmetries associated with the 1D KPZ equation, the fluctuation–dissipation relation and Galilean invariance, we have found a couple of relevant

results. It is clear that both these symmetries are recovered when taking the continuum limit of any reasonable discretization scheme. And thus, an accurate enough partition must yield suitable results.

The fluctuation–dissipation relation essentially tells us that the nonlinearity is not operative in 1D and for long times. Our analysis indicates that the problem with the fluctuation–dissipation theorem in  $1 + 1$  can be circumvented by improving the numerical accuracy. Or this is at least what would happen if the interface were smooth enough. We are not completely free of surprises coming from the irregular nature of rough interfaces (as we already mentioned we expect a Hölder exponent strictly smaller than  $1/2$  for  $d$ –dimensional KPZ interfaces). In any case, our simulations have indicated that our strategy of improving the numerical accuracy yields operative results.

Galilean invariance has been always associated with the exactness of the 1D KPZ exponents, and with a relation that connects the critical exponents in higher dimensions. However, it is worth remarking that this interpretation has been recently criticized [24]. Our analysis indicates that if the numerical solution obtained with a finite differences scheme that is not Galilean invariant yields the well known critical exponents, that would strongly suggests that Galilean invariance is not a fundamental symmetry as usually considered. It is worth commenting that the results presented here for different *consistent* discretization schemes show all the same critical exponents as the standard one, Eq. (42).

Here we remark that in the present work we have only emphasized the existing constraints introduced by the local transformation on the discrete versions of the differential equations. No attempt is made here of choosing the most suitable spatial discretization scheme with regard to a given KPZ feature, nor to present a deep analysis of results regarding the violation of Galilean invariance. The study of such aspects, together with the evaluation of the effects of the relations obtained among the discrete operators on different relevant quantities as well as other problems will be the subject of further work.

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